Methyl salicylate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 234 °C

Global applicability domain: Inside

Local applicability domain index: 7.42e-01

Confidence level: 8.57e-01

Nearest Neighbors from the Training Set

Image not found
1-Phenoxy-2-propanol
Measured: 243
Predicted: 244

Image not found
2-Phenoxy-1-propanol
Measured: 244
Predicted: 244

Image not found
Methyl salicylate
Measured: 223
Predicted: 234

Image not found
2-Allylphenol
Measured: 220
Predicted: 233

Image not found
Chavicol
Measured: 238
Predicted: 231